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The SER-CAT Virtual Beamline: Providing Light when You Need it in Your Home Lab

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Since 1999, SER-CAT has been working towards the concept of providing its members with a “*Virtual Beamline*”, which could be integrated into their daily workflow much like your X-ray lab down the hall.

We began investigating robotic crystal mounting automation in 2000 with Oceaneering Space Systems. In 2003, a highly modified Berkeley ALS Automounter was installed on 22BM. Using 22BM as a user-based testbed, the beamline and experiment control interface *SERGUI* was continually modified until a reliable, robust and user-friendly system was achieved. In 2006, the SER-CAT *Virtual Beamline* came online providing remote crystal screening and data collection capability on both 22ID (capacity 450 crystals) and 22BM (capacity 96 crystals).

The *SERGUI* beam line control interface allows the direct remote access of SER-CAT beamline from their home labs including : 1) beamline/goniometer optimization, 2) wavelength selection, 3) fluorescence scans, 4) automatic crystal centering and rastering, 5) automated crystal screening, 6) MAD/SAD/Helical data collection and others. Today over 95% of SER-CAT members routinely collect data remotely. SER-CAT has also implemented 12-hour shifts with 16-hours/day and 7-days/week of on-site user support to assist users for their remote accesses from home labs. Multiple Access Time (MAT) shifts have also been made available to SER-CAT members for fast turn-around and flexible data collection capabilities.

SER-CAT also provides its members the on-the-fly automated data processing using XDS, KYLIN and DIALS. HKL2000, XDS, MOSFLM, and DIALS for manual data processing. All user data can be remotely, quickly, reliably and securely downloaded from SER-CAT's Globus/GridFTP archive server to the users' home systems anywhere and anytime.

During the annual SER-CAT Symposium, awards are given out to recognize senior investigator's “Outstanding Science” and young investigator's “Outstanding Research Achievement” carried out at SER-CAT.

1. Introduction

The SouthEast Regional Collaborative Access Team (SER-CAT) (<https://www2.ser.aps.anl.gov>) is a consortium formed to provide third generation X-ray capabilities to macromolecular crystallographers and structural biologists of its membership institutions. SER-CAT is located at Advanced Photon Source, Argonne National Laboratory outside Chicago. It is operated by the University of Georgia and currently has 19 Membership institutions and 4 associate members located across the East Coast, the South and the Midwest regions of the United States (Fig.1).

SER-CAT's path to making its “Virtual Beamline” a reality started more than 20 years ago. In 1999, SER-CAT conceived the concept of providing its members with a “Virtual Beamline for their Home Labs”, which could be

integrated into their daily work flow much like the X-ray lab down the hall. SER-CAT beamlines, 22ID and 22BM, were designed and built for this purpose from the beginning. In 2000, working with the Oceaneering Space System a conceptual design of an ASTRo Automounter prototype was developed (Fig.2) but delayed since the completion of SER-CAT's first beamline (scheduled for 2002) was the highest priority. In 2003, after considerable discussions, SER-CAT selected the ALS-Berkeley automounter. Together with improved, in-house designed sample Dewars, an automated crystal mounting system with remote access capability was constructed and installed on beamline 22BM for commissioning and testing and later on the beamline 22ID with a two-Dewar system (Fig.3).

Today, the SER-CAT “Virtual Beamline” is mature and robust with 95% of all SER-CAT data being collected

Fig.1 SER-CAT Membership and Associate User Institutions.

Fig.2 The OSS ASTRo Automounter prototype.

Fig.3 The SER-CAT modified Berkley-ALS style automounter installed on beamline 22ID.

remotely. SER-CAT's home grown SERGUI (see below) user interface provides full beamline control for data collection, whether local or remote. To support more efficient beamline usage, SER-CAT offers standard 12-hour user shifts and 16-hour staff support to all remote users. In cases where fast turnaround is needed, flexible Multi-User Access Time (MAT) is available to SER-CAT members every week. The "Virtual Beamline" has greatly improved data collection productivity. During the past 5 years 22ID users have screened more than 134 K crystal samples and collected more than 67 K data sets, which is about 129 crystals screened and 65 data sets collected per APS beam operation day.

SER-CAT hosts two fully automated beamlines, 22ID an Undulator A insertion device (ID) beamline, and 22BM a bending magnet (BM) beamline. Both beamlines have an energy range between 6 keV - 20 keV producing Si(111) monochromated X-rays. 22ID has full beam flux at 12 keV of 8×10^{12} photons/second, with a beam size (FWHM) of $20 \times 30 \mu\text{m}$ that was achieved by both sagittal focus and elliptical focus by the horizontal mirror of a mini K-B mirror system, installed in 2018. The full K-B mirror system would be installed during SER-CAT and APS upgrade period starting 2022. 22BM has full beam flux at 12 keV of $1.3 \times$

10^{11} photons/second, with a beam size (FWHM) is $90 \times 90 \mu\text{m}$. Both beamlines are equipped with fast detectors, with a Dectris Eiger X16M 133 MHz HPAD detector on 22ID and 10 MHz Rayonix MX300HS CCD detector on 22BM (Fig.4). Both detectors support shutterless-data collection that significantly increases the speed of data collection and the quality of the data produced. Both beamlines support MAD and SAD phasing (including Native SAD and long wavelength SAD experiments). Since the ALS-Berkeley automounter was installed on 22BM in 2003, it has been continuously upgraded. The highly reliable automounter on 22ID can hold up to 450 samples (2 Dewars, each with a 225-sample capacity) at one time, designed to accommodate the pucks of multiple users scheduled for different time slots during the day. The large capacity system makes it possible to have smooth and quick transitions between different remote users without having to stop frequently to make puck changes.

To make remote access simple and user friendly the "Virtual Beamline" provides all tools available to on-site users, as well as the same SERGUI user interface. This gives the remote user full control of the beamline from their

22ID Technical Specifications		22ID Configurations	
Insertion Device:	undulator A	Robotic system:	2 large dewars (450)
Energy range:	6 ~ 20 Kev	Detector:	Dectris Eiger 16M
Monochromator:	Si (111)	Goniometer:	MD2 diffractometer
Beam size:	20 x 30 μm (FWHM)	Applications:	MAD, SAD
Horizontal focus:	sagittal + elliptical mirror		sample screening
Vertical focus:	elliptically bent mirror		shutterless collection
Full beam flux @ 12 Kev:	8×10^{12} (photons/sec)		extended wavelength

22BM Technical Specifications		22BM Configurations	
No Insertion Device:	bending magnet	Robotic system:	1 dewar (96)
Energy range:	6 ~ 20 Kev	Detector:	Rayonix MX300HS
Monochromator:	Si (111)	Goniometer:	single Phi stage
Beam size:	90 x 90 μm (FWHM)	Applications:	MAD, SAD
Horizontal focus:	sagittal + elliptical mirror		sample screening
Vertical focus:	elliptically bent mirror		shutterless collection
Full beam flux @ 12 Kev:	1.3×10^{11} (photons/sec)		long wavelength.

22ID Compact KB Mirror System		Beamline Data Storage System	
Substrate:	Trapezoidally Cut Si	Panasas PanFS file system:	485 TB
Surface coating:	Rh	Data Archive:	2 years
Length:	320 mm	Data Transfer:	GridFTP
Surface roughness:	< 1 Å	Data Security:	LDAP server
Slope errors:	< 0.1 μradian		

Fig.4 Beamline Specifications, Configurations and Data Storage.

home lab, including beamline optics for energy change and optimization, motion control for motor movement, robotics for crystal mounting, and goniometry (MD2 diffractometer) for sample alignment. The SERGUI supports multi-detector platforms allowing the detectors to be quickly swapped in the case of a detector failure to reduce beamline downtime. Different data collection strategies (MAD, SAD or high resolution) can be easily set up, and auto-data processing running in the background is also available. APS ring status including ring current etc. is displayed real-time on SERGUI's status bar. These tools running under the SERGUI user interface gives the remote user the same feeling and controls that SER-CAT staff and local users would have while collecting data on-site. In essence, all the remote user needs is a laptop with a good internet connection and a phone to call beamline staff for help if needed.

To support secure remote access, the SER-CAT remote access portal has servers running both NX (nomachine.com) and X2GO (wiki.x2go.org) remote access clients. Users just simply downloads either the NX or X2GO client (both are free) for their preferred platforms (Linux, Windows or Mac) and they are ready to go. The secure remote connections are made via SSH or NX protocols. Beamline access is controlled by an LDAP (Lightweight Directory Access Protocol) server which provides scheduled access to the beamline control and data processing computers used for data collection. The same user credentials can also be used to access other SER-CAT resources for further data processing and structure determination at any time. Finally, the remote sessions can be monitored by beamline staff any time day or night. This feature provides a very useful tool for the staff to diagnose

and fix the problems remote users may encounter either with the instrument or software.

2. SERGUI

The Python-based SERGUI user interface was developed in house by SER-CAT in 2003, and has been continuously upgraded ever since. SERGUI functions as the brain of the beamline operation, while providing a user interface, operating motion controllers, optimizing beamline optics, crystal mounting and alignment, and conducting data collection and data processing. (Fig.5a). The program is organized into several defined areas: (1) Data Management and Logbook, (2) Hutch, (3) Sample, (4) MAD, and (5) Collect and Screen panels (Fig.5a, b).

The SERGUI Log Panel

Using the Logbook panel (Fig.5b), beamline users can easily upload a pre-prepared sample file (csv format) containing puck and pin information for each sample in the puck. Access to this information is controlled by the LDAP server so each user can only see and operate on their own pucks. SERGUI can automatically create all the necessary directories for each sample, including a test directory for single images, an images directory for the data set, and a process directory for auto-data processing results. This feature makes data navigation much easier since remote users can focus on experiment instead of tedious and error prone book keeping.

The SERGUI Hutch Panel

Using the Hutch panel (Fig.6), beam energy or wavelength can be changed, and the beamline automatically optimized (X-ray optics, MD2 table and beam shaping pin holes) to

Fig.5a SERGUI and Beamline Control.

Fig.5b SERGUI interface.

Fig.6 SERGUI – Hutch Panel.

get the maximum beam intensity on the sample. Changing beam energy and beamline optimization are very easy to do and straight forward. SER-CAT remote users routinely change energy back and forth independently for different types of experiments. The APS ring current and hutch status are displayed at the bottom of SERGUI user interface. Users can remotely operate all the shutters, which are also under the control of the APS safety interlock systems. Diffraction images are automatically streamed to the ADXV image display program for display and inspection. The image refresh rate is 1 HZ. This defines which images are shown.

The SERGUI Sample Panel

Once the beam energy has been changed and the beamline

has been optimized and aligned the Sample Panel (Fig.7) is used to dismount, mount and align the crystalline samples. Crystals may be manually centered using two-click centering, automatic loop centering and raster scanning (Song, Mathew *et al.* 2007). Pinholes (50 – 10 μm) can be selected to match the beam size with crystal size. The dismount-mount-align process using automated loop centering is approximately 1 minute. Raster scanning is useful for tiny or hard to see crystals. The rastering scanning process uses a series of low dose exposures covering a defined region of the loop. Three beam sizes (10-, 20- and 50-microns are available to allow the user to match the beam size to the raster size).

The rastered images are then analyzed for the number and

Fig.7 SERGUI – Sample Panel, showing a raster grid for X-ray sample centering.

Fig.8 SERGUI – Helical Data Collection.

intensity of spots observed and the crystal is then centered at the point giving the maximum spot count. Rastering can be carried out in one, two or three dimensions, and the whole process takes about one minute. Three dimensional rastering forms the basis for helical data collection (Flot, Mairs *et al.* 2010) on radiation sensitive crystals or thin needles where the X-ray dose can be spread over the length of the crystal. Here the user defines two end points on the crystal which defines the helical axis (Fig.8). During data collection the crystal is then rotated and translated along the helical axis spreading out the X-ray dose.

The SERGUI MAD Panel

MAD experiments can be set up using the MAD panel (Fig.9). Users can simply select the anomalous scatterer from the Periodic Table, pick an absorption edge, change

beamline energy, optimize the beam and carryout a fluorescence scan on the crystal. SERGUI running Benny-Chooch analysis (Evans and Pettifer 2001) on the scan calculates the f' and f'' values at the peak, inflection, and remote points, which are then used to automatically set-up the MAD experiment.

The SERGUI Collect Panel

Using the Collect page, (Fig.10) user can collect a single image, set up native or helical data collection and SAD or MAD experiments. If needed, SERGUI can also provide a data collection strategy for the experiment. Auto-processing running in the background begins automatically once data collection begins. All meta data related to the experiment is automatically recorded in the beamline database. For the Eiger 16M, normal data collection frame rates range between

Fig.9 SERGUI – MAD Panel.

Fig.10 SERGUI – Collect Panel.

5 Hz to 20 Hz, with a maximum frame rate of 50 Hz. The normal scan width is 0.25 degrees, with a majority of data sets finishing in one to two minutes. In the case of MAD data collection, data sets can be set up at different wavelengths, with SERGUI providing options for inverse beam (Hendrickson, Pahler *et al.* 1989) or wedging (Derewenda and Helliwell 1989).

The SERGUI Screening Panel

Since the data collection has become so fast, remote data collection has become almost mechanical: dismount-mount samples, align sample, take screening shots, evaluate the images, set up data collection, run data reduction, etc. The result is that remote data collection has become repetitive and tedious. Auto-screening and auto-data collection using SERGUI (Fig.11) would address this problem in addition to making crystal screening more efficient. Here, the user can define which of their samples they wish to have screened and other criteria. These samples would then be automatically mounted, centered; and screening images taken and indexed. Promising samples would then be marked for auto-data collection following user defined protocols.

SER-CAT Automated Data Reduction

The automated data processing system introduced in 2007 and updated continually since then is designed to reduce the data on-the-fly during data collection. Currently it runs parallel jobs using three different data reduction packages: XDS (Kabsch 2010), DIALS (Winter, Waterman *et al.* 2018) and locally developed KYLIN package. Results from the auto-processing will be deposited in the user's process directory. These calculations are carried out on SER-CAT's

computing cloud which includes a 108-processor Linux cluster and an additional 206 cloud-based processors from multiple workstations. In most cases, auto-processing will complete in a few minutes after the data collection finishes. In addition, a complete suite of data processing packages HKL2000 (Minor and Otwinowski 1997), XDS, MOSFLM (Battye, Kontogiannis *et al.* 2011), KYLIN or DIALS are also available for users who wish to process or reprocess their data manually.

By the end of the remote access session, users will have three log files in their data directory, a robot sample mounting log, a log of data sets collected and a log of auto-data processing results. The robot sample mounting log contains a record of all mounted sample IDs and a time stamp of the sample mounting. The data set log has the full record of all data set parameters, including sample ID, time of data collection, wavelength and transmission, exposure time and scan width, scan range, distance, beam intensity, detector type, beamline ID, user and group ID, etc. More importantly, the information about data sets collected and their reduction statistics is extremely helpful in gauging the productivity and quality of the data collection. The auto-data processing log gives the useful summary of the results from each of the data reduction packages such as R-merge, resolution, completeness, redundancy, I/sigma, unit cell, space group, mosaicity and others. Based on this information, the user may move on to the next level solving the crystal structure, or go back to reprocess the data for certain data sets.

SER-CAT Data Management

Fast data collection has generated a huge demand for high-

Fig.11 SERGUI – Automatic Data Screening Panel.

Fig.12 Participants at 2019 SER-CAT Symposium.

Table 1 SER-CAT Outstanding Science Awards and Young Investigator Awards Winners.

Outstanding Award Winners			Young Scientist Award Winners		
2020	Dr. Pei Zhou	Duke University School of Medicine	2019	Ms. Stephanie Bester	University of Georgia
2020	Dr. Gary J. Nabel	Sanofi Research and Development	2019	Mr. Andres Wong-Sam	Georgia State University
2019	Dr. Jacek Lubkowski	NCI, NIH	2018	Dr. Emily Weikum	Emory University
2018	Dr. Seok-Yong Lee	Duke University School of Medicine	2017	Mr. William Bradley O'Dell	North Carolina State University
2017	Dr. Jochen Zimmer	University of Virginia	2016	Mr. Marc Schureck	Emory University
2016	Dr. Paul Shaffer	Amgen, Inc.			
2015	Dr. Xiaodong Cheng	Emory University			
2014	Dr. Samuel H. Wilson	NIEHS, NIH	2014	Dr. Edward Pryor	University of Virginia
2013	Dr. Susan Buchanan	NIAID, NIH	2013	Dr. Matthew J. Schellenberg	NIEHS, NIH
2012	Dr. Peter D. Kwong	NIAID, NIH	2012	Dr. Jason Stagno	NCI, NIH
2011	Dr. Fred Dyda	NIDDK, NIH	2011	Mr. Stefan Gajewski	St. Jude Children's Research Hospital
2010	Dr. Xinhua Ji	NCI, NIH			
2009	Dr. James Hurley	NIDDK, NIH	2009	Mr. Guoxing Fu	Georgia State University
2008	Dr. Dmitry Vassilyev	University of Alabama at Birmingham	2008	Dr. Da Jia	Emory University
2007	Dr. Michael Wiener	University of Virginia	2007	Dr. Ping Liu	Georgia State University
2006	Dr. Bin Zhao	Vanderbilt University Medical Center	2006	Dr. Jianhua Gan	NCI, NIH
2005	Dr. Lorena Beese	Duke University	2005	Dr. Nicole LaRonde-LeBlanc	NCI, NIH

performance Enterprise data storage. To meet this demand, SER-CAT hosts a Panasas Enterprise file system on-site. The Panasas file system is a network attached storage (NAS) appliance that integrates hybrid storage hardware and the proprietary PanFS parallel file system for fast data access. This system provides a total of 465 TB data storage for SER-CAT's two beamlines, allowing data to be archived up to two years (Fig.4). Security and privacy of users' data are always SER-CAT top priority. The beamline LDAP server controls and safeguards user's access to only the data they own in the archive. Secure point-to-point data transfer from SER-CAT to the user's home laboratory is facilitated using Globus/ GridFTP data transfer protocol. Data transfer is provided by a dedicated network from Argonne National Laboratory to the outside without interfering with the local beamline network. Thus, as long as user can access the internet and web browser from anywhere at any time, they can start a data transfer.

3. The SER-CAT User Community, Annual Meetings and Science Awards

In 1997, a group of scientists from the southeast region of the U.S. came together at the University of Georgia to explore the possibility of obtaining dedicated beamline access for single crystal diffraction experiments for their projects. From this meeting the SER-CAT community was born, with the intent of building a state-of-the-art facility for X-ray Structural Biology at the Advanced Photon Source, Argonne National Laboratory as a "shared research resource" for institutions in the state of Georgia and its neighboring states.

The Georgia Research Alliance (<https://gra.org>) provided matching funds for beamline construction for the universities in Georgia.

Since the SER-CAT facility was located hundreds of miles from most SER-CAT institutions an annual Symposium held at a membership Institution was begun. The intent of the Symposium was to bring SER-CAT to its users and to highlight SER-CAT research and technical advances. The first SER-CAT Symposium was held in 2005. Fig.12 shows the meeting participants at the most recent in-person 2019 Symposium hosted by the University of Alabama at Birmingham. During each annual symposium, awards were given (based on a publication from the previous year) to recognize the "Outstanding Science" carried out at SER-CAT and outstanding research achievement by "Young Investigator" (post doc or graduate student). A list of SER-CAT Outstanding Science Award winners and Young Investigator Awards can be found in Table 1.

For those interested in using the SER-CAT Virtual Beamline contact one of the authors.

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